Numerical simulation of a Controlled-Controlled-Not (CCN) quantum gate in a chain of three interacting nuclear spins system

G.V. López and L. Lara
Departamento de Física, Universidad de Guadalajara
Apartado Postal 4-137, 44410 Guadalajara, Jalisco, México

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ABSTRACT

We present the study of a quantum Controlled-Controlled-Not gate, implemented in a chain of three nuclear spins weakly Ising interacting between all of them, that is, taking into account first and second neighbor spin interactions. This implementation is done using a single resonant π-pulse on the initial state of the system (digital and superposition). The fidelity parameter is used to determine the behavior of the CCN quantum gate as a function of the ratio of the second neighbor interaction coupling constant to the first neighbor interaction coupling constant (J'/J). We found that for $J'/J \geq 0.02$ we can have a well defined CCN quantum gate.

1. Introduction

There is not doubt that the discovery of the polynomial time solution of the prime factorization problem (Shor's algorithm [1]) and the fastest data base searching (Grover's algorithm [2]) by a quantum computer, and the importance of the implementations of these algorithms in cryptography analysis [3] have made the study of the physical realization of a quantum computer a priority for many researcher [4,5]. A quantum computer works with qubits instead of bit, where a qubit is the superposition of two quantum levels of the system which are defined as $|0\rangle$ and $|1\rangle$, and a tensorial product of these states makes up a register. Although, one could say that there are already quantum computers with registers of few qubits [6], these are still far too low to make serious studies (which may require at least 100-qubits registers, that is, at least a 2^{100} dimensional Hilbert space). In addition, Much more technology development (or very neat idea) is needed to have a real powerful quantum computer. One model of solid state quantum computer which looks promising due to advances in single spin measurements [7] is that of a chain of nuclear spins quantum computer [4,8], where the Ising interaction between first neighbor is considered. This interaction allows us to implement ideally this type of computer up to 1000 qubits or more [9]. First neighbor interaction between spins also allows to implement a Controlled-Not (CN) quantum gate using a single π-pulse [10]. However, the implementation of a Controlled-Controlled-Not (CCN) quantum gate, which is needed in Shor's factorization, Grover's searching and Full-Adder algorithms [11], is not that simple. In addition, CCN quantum gate is also important since it has universality characteristic [12]. The CN and CCN gates are defined classically by the following two tables [13]

CN			
a	b	a'	b'
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

Table 1

CCN					
a	b	c	a'	b'	c'
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	0	1
1	1	0	1	1	1
1	1	1	1	1	0

Table 2

where a (called control bit) and b (called target bit) for CN (a,b and c for CCN) represent the input information, and a' and b' (a', b', and c' for CNN) represent the output information. In a CN gate, "b'" (target) changes if an only if "a"(control) has the value 1. In a CCN gate, "c'" changes if an only if "a" and "b" has the value 1. The ideals CN and CCN quantum gates, operating on an arbitrary L-register $|i_{L-1},\dots,i_a,\dots,i_b,\dots,i_c,\dots,i_0\rangle$ (where $i_j=0,1$), would be defined as

$$CN_{ab}|i_{L-1},\dots,i_a,\dots,i_b,\dots,i_c,\dots,i_0\rangle = |i_{L-1},\dots,i_a,\dots,i_b\oplus i_a,\dots,i_c,\dots,i_0\rangle$$

and

$$CCN_{abc}|i_{L-1},\dots,i_a,\dots,i_b,\dots,i_c,\dots,i_0\rangle = |i_{L-1},\dots,i_a,\dots,i_b,\dots,i_c\oplus(i_a\cdot i_b),\dots,i_0\rangle\ ,$$

where the operation $\oplus$ means summation module 2. In this paper we show that considering second neighbor interaction between spins in the one-dimensional chain of spins quantum computer, and we show that it is possible to implement a CCN quantum gate with just a single π-pulse. Of course, a CN quantum gate continue being represented by a single π-pulse.

2. Equation of Motion

Consider a one-dimensional chain of three equally spaced nuclear-spins system (spin one half) making an angle $\cos\theta=1/\sqrt{3}$ with respect the z-component of the magnetic field (chosen in this way to kill the dipole-dipole interaction between spins) and having an rf-magnetic field in the transversal plane. The magnetic field is given by

$$\mathbf{B}=(b\cos\omega t,-b\sin\omega t,B(z))\ , \tag{1}$$

where b is the amplitude of the rf-field, $B(z)$ is the amplitude of the z-component of the magnetic field, ω is the angular frequency of the rf-field (its phase has been chosen as zero for simplicity). So, the Hamiltonian of the system is given by

$$H=-\sum_{k=0}^{2}\mu_{\mathbf{k}}\cdot\mathbf{B}_{\mathbf{k}}-2J\hbar\sum_{k=0}^{1}I_k^zI_{k+1}^z-2J'\hbar\sum_{k=0}^{0}I_k^zI_{k+2}^z\ , \tag{2}$$

where $\mu_{\mathbf{k}}$ represents the magnetic moment of the kth-nucleus which is given in terms of the nuclear spin as $\mu_{\mathbf{k}}=\hbar\gamma(I_k^x,I_k^y,I_k^z)$, being γ the proton gyromagnetic ratio. $\mathbf{B}_{\mathbf{k}}$ represents the magnetic field at the location of the kth-spin. The second term at the right side of (2) represents the first neighbor spin interaction, and the third term represents the second neighbor spin interaction. J and J' are the coupling constants for these interactions. This Hamiltonian can be written in the following way

$$H=H_0+W\ , \tag{3a}$$

where H_0 and W are given by

$$H_0=-\hbar\left\{\sum_{k=0}^{2}\omega_kI_k^z+2J(I_0^zI_1^z+I_1^zI_2^z)+2J'I_0^zI_2^z\right\} \tag{3b}$$

and

$$W = -\frac{\hbar\Omega}{2}\sum_{k=0}^{2}\left[e^{i\omega t}I_k^{+} + e^{-i\omega t}I_k^{-}\right] . \tag{3c}$$

Here, $\omega_k = \gamma B(z_k)$ is the Larmore frequency of the kth-spin, $\Omega = \gamma b$ is the Rabi's frequency, and $I_k^{\pm} = I_k^x \pm iI_k^y$ represents the ascend operator (+) or the descend operator (-). The Hamiltonian H_0 is diagonal on the basis $\{|i_2 i_1 i_0\rangle\}$ with $i_j = 0, 1$ (zero for the ground state and one for the exited state),

$$H_0|i_2 i_1 i_0\rangle = E_{i_2 i_1 i_0}|i_2 i_1 i_0\rangle . \tag{4a}$$

The eigenvalues $E_{i_2 i_1 i_0}$ are given by

$$E_{i_2 i_1 i_0} = -\frac{\hbar}{2}\left\{(-1)^{i_2}\omega_2 + (-)^{i_1}\omega_1 + (-1)^{i_0}\omega_0 + J[(-1)^{i_0+i_1} + (-1)^{i_1+i_2}] + (-1)^{i_0+i_2}J'\right\} . \tag{4b}$$

The term (3c) of the Hamiltonian (3a) allows to have a single spin transitions on the above eigenstates by choosing the proper resonant frequency, as shown in Figure 1. For example, if we are interested in having the transition $|110\rangle \longleftrightarrow |111\rangle$ since this one represents the CCN quantum gate operation, according with the table 2, the resonant frequency would be

$$\omega = \omega_0 - J - J' . \tag{5}$$

Of course, we could also have considered a CCN quantum gate as defined by the transition $|011\rangle \longleftrightarrow |111\rangle$, by defining the order of the elements differently.

To solve the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi , \tag{6}$$

let us propose a solution of the form

$$\Psi(t) = \sum_{k=0}^{7} C_k(t)|k\rangle , \tag{6}$$

where we have used decimal notation for the eigenstates in (4a), $H_0|k\rangle = E_k|k\rangle$. Substituting (6) in (5), multiplying for the bra $\langle m|$, and using the orthogonality relation $\langle m|k\rangle = \delta_{mk}$, we get the following equation for the coefficients

$$i\hbar\dot{C}_m = E_m C_m + \sum_{k=0}^{7} C_k\langle m|W|k\rangle \quad m = 0, \ldots, 7. \tag{7}$$

Now, using the following transformation

$$C_m = D_m e^{-iE_m t/\hbar} , \tag{8}$$

the fast oscillation term $E_m C_m$ of Eq. (7) is removed (this is equivalent to going to the rotating frame of reference), and the following equation is gotten for the coefficients D_m

$$i\dot{D}_m = \frac{1}{\hbar}\sum_{k=0}^{7} W_{mk}D_k e^{i\omega_{mk}t} , \tag{9a}$$

where W_{mk} denotes the matrix elements $\langle m|W|k\rangle$, and ω_{mk} are defined as

$$\omega_{mk} = \frac{E_m - E_k}{\hbar} \ . \tag{9b}$$

Eq. (9a) represents a set of sixteen real coupling ordinary differential equations which can be solved numerically, and where W_{mk} are the elements of the matrix

$$(W) = -\frac{\hbar\Omega}{2}\begin{pmatrix} 0 & z^* & z^* & 0 & z^* & 0 & 0 & 0 \\ z & 0 & 0 & z^* & 0 & z^* & 0 & 0 \\ z & 0 & 0 & z^* & 0 & 0 & z^* & 0 \\ 0 & z & z & 0 & 0 & 0 & 0 & z^* \\ z & 0 & 0 & 0 & 0 & z^* & z^* & 0 \\ 0 & z & 0 & 0 & z & 0 & 0 & z^* \\ 0 & 0 & z & 0 & z & 0 & 0 & z^* \\ 0 & 0 & 0 & z & 0 & z & z & 0 \end{pmatrix} \ , \tag{9c}$$

where z is defined as $z = e^{i\omega t}$, and z^* is its complex conjugated.

3. Numerical Simulations

To solve numerically (9a), we shall use similar values for the parameters as reference (9). So, in units of $2\pi \times MHz$, we set the following values

$$\omega_0 = 100 \ , \ \omega_1 = 200 \ , \ \omega_2 = 400 \ , \ J = 5 \ , \ \Omega = 0.1 \tag{10}$$

The coupling constant J' is chosen with at least one order of magnitude less that J since in the chain of spins one expects that second neighbor contribution to be at least one order of magnitude weaker than first neighbor contribution. We consider digital initial state and superposition initial states,

$$\Psi(0) = |110\rangle \tag{10a}$$

and

$$\begin{aligned}\Psi(0) \quad = \quad & \frac{2}{3\sqrt{8}}|000\rangle + \frac{\sqrt{14}}{3\sqrt{8}}|001\rangle + \frac{1}{3\sqrt{8}}|010\rangle + \frac{\sqrt{17}}{3\sqrt{8}}|011\rangle \\ & + \frac{3}{4\sqrt{8}}|100\rangle + \frac{\sqrt{23}}{4\sqrt{8}}|101\rangle + \frac{1}{2\sqrt{8}}|110\rangle + \frac{\sqrt{7}}{2\sqrt{8}}|111\rangle \ ,\end{aligned} \tag{10b}$$

to cover all the important aspects of the CNN quantum gate. In all our simulations the total probability, $\sum |C_k(t)|^2$, is conserved equal to one within a precision of 10^{-6} (note that $|C_k| = |D_k|$). Figure 2 shows the behavior of $Re\ D_6$, $Im\ D_6$, $Re\ D_7$ and $Im\ D_7$ during a π-pulse ($t = \tau = \pi/\Omega$) for the digital initial state and with $J' = 0.1$. One can see clearly the transition $|110\rangle \longrightarrow i|111\rangle$, defining the CCN quantum gate up to a global phase ($\pi/2$). Figure 3a shows the behavior of the probabilities $|C_k|$ for $k = 0, \ldots, 7$ during a π-pulse for the superposition initial state and with $J' = 0.1$ and for the superposition initial condition. Figure 3b shows the behavior of the

expected value of the z-component of the spin, $\langle I_k^z \rangle$, k=0,1,2, during a π-pulse with the initial superposition state and $J' = 0.1$. These expected values are given by

$$\langle I_0^z \rangle = \frac{1}{2} \sum_{k=0}^{7} (-1)^k |C_k(t)|^2 \ , \tag{11a}$$

$$\langle I_1^z \rangle = \frac{1}{2} \Big\{ |C_0|^2 + |C_1|^2 - |C_2|^2 - |C_3|^2 + |C_4|^2 + |C_5|^2 - |C_6|^2 - |C_7|^2 \Big\} \ , \tag{11b}$$

and

$$\langle I_2^z \rangle = \frac{1}{2} \sum_{k=0}^{3} |C_k|^2 - \sum_{k=4}^{7} |C_k|^2 \ . \tag{11c}$$

As one could expect, only the spin related with the first qubit (having subindex zero) changes its value at the end of the π-pulse. The behavior of the expected values of the x and y components of the spin, $\langle I_k^x \rangle$ and $\langle I_k^y \rangle$ for $k = 0, 1, 2$, is shown on Figure 4 for the superposition initial state and for $j' = 0.1$. These expected values are given by

$$\langle I_0^x \rangle = Re\Big(C_1^* C_0 + C_3^* C_2 + C_5^* C_4 + C_7^* C_6 \Big) \ , \qquad \langle I_0^y \rangle = Im\Big(\dots \Big) \ , \tag{12a}$$

$$\langle I_1^x \rangle = Re\Big(C_2^* C_0 + C_3^* C_1 + C_6^* C_4 + C_7^* C_5 \Big) \ , \qquad \langle I_1^y \rangle = Im\Big(\dots \Big) \ , \tag{12b}$$

and

$$\langle I_2^x \rangle = Re\Big(C_4^* C_0 + C_5^* C_1 + C_6^* C_2 + C_7^* C_3 \Big) \ , \qquad \langle I_2^y \rangle = Im\Big(\dots \Big) \ . \tag{12c}$$

The fast oscillations appearing on this behavior are due to the time depending phases in Eq. (8) which have these terms and which are not cancelled out.

For the case $J' = 0$, the resonant frequency for the transition $|110\rangle \longleftrightarrow |111\rangle$ and the transition $|010\rangle \longleftrightarrow |011\rangle$ coincides and both transitions appears in the dynamics of the system (simultaneous CN and CCN operations). Thus, the question which arises is: what is the minimum value of J' which allows to have a well define CCN quantum gate ? To answer this question, Fig. 5 (a) and (b) shows the behavior of the CN quantum gate with the resonant frequency of the CCN quantum gate ($\omega = \omega_0 - J - J'$) during a π-pulse for several J' values. In addition, (c) and (d) show the fidelity [14], $F = \langle \Psi_{expected} | \Psi(\tau) \rangle$, associated to CCN quantum gate as a function of J'/J. As one can see from these figures, with J' values of even two orders of magnitude ($J'/J = 0.02$) we can already have a very well defined CCN quantum gate. Therefore, it is very likely that a single pulse CCN quantum gate can be implemented in a chain of nuclear spin quantum computer.

4. Conclusions and comments

We presented the study of a Controlled-Controlled-Not (CCN) quantum gate implemented in a chain of nuclear spins weakly Ising interacting and with the use of

a single π-pulse. With study this gate with digital and superposition initial states and found an expected global phase for its definition,

$$\begin{aligned} \widehat{CCN} &= |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |011\rangle\langle 011| + |100\rangle\langle 100| \\ &+ |101\rangle\langle 101| + i|110\rangle\langle 111| + i|111\rangle\langle 110| \ . \end{aligned} \tag{13}$$

Using the fidelity parameter, we have seen that it is very likely to have the implementation of a CCN quantum gate in the chain of nuclear spin quantum computer since the coupling constant to second neighbor interaction can be even two order of magnitude lower than the first neighbor interaction, and still having a well defined CCN quantum gate. Since the eigenvalues in (4a) depends on J', Eq. (4b), the detuning factor, defined as $\Delta = (E_p - E_m)/\hbar - \omega$ for the transition $|p\rangle \longleftrightarrow |m\rangle$ (decimal notation), will depends also on J'. Therefore, the normal 2πk-method used in reference (8) will have to change correspondently to be able to suppress non-resonant transitions in multiple-pulses algorithms.

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Figure Captions

Fig. 1 Energy levels and resonant frequencies.

Fig. 2 CCN quantum gate with digital initial condition and with $J' = 0.1$. (1):$Re\ D_6$, (2):$Im\ D_6$, (3):$Re\ D_7$, (4):$Im\ D_7$.

Fig. 3 For the superposition initial state and for $J' = 0.1$, (a) Probabilities $|C_k(t)|^2$ for $k = 0, \ldots, 7$. (b) Expected values (0): $\langle I_0^z \rangle$, (1): $\langle I_1^z \rangle$, and (2): $\langle I_2^z \rangle$.

Fig. 4 For the superposition initial state and for $J' = 0.1$, expected values of the transversal components of the spin.

Fig. 5 For the superposition initial condition. (a) Probability $|C_2|^2$, and (b) Probability $|C_3|^2$ for (1): $J' = 0.0$, (2): $J' = 0.02$, (3): $J' = 0.04$, (4): $J' = 0.06$, (5): $J' = 0.08$, and (6): $J' = 0.1$. (c) Real and Imaginary parts of the Fidelity. (c) Modulus of Fidelity.

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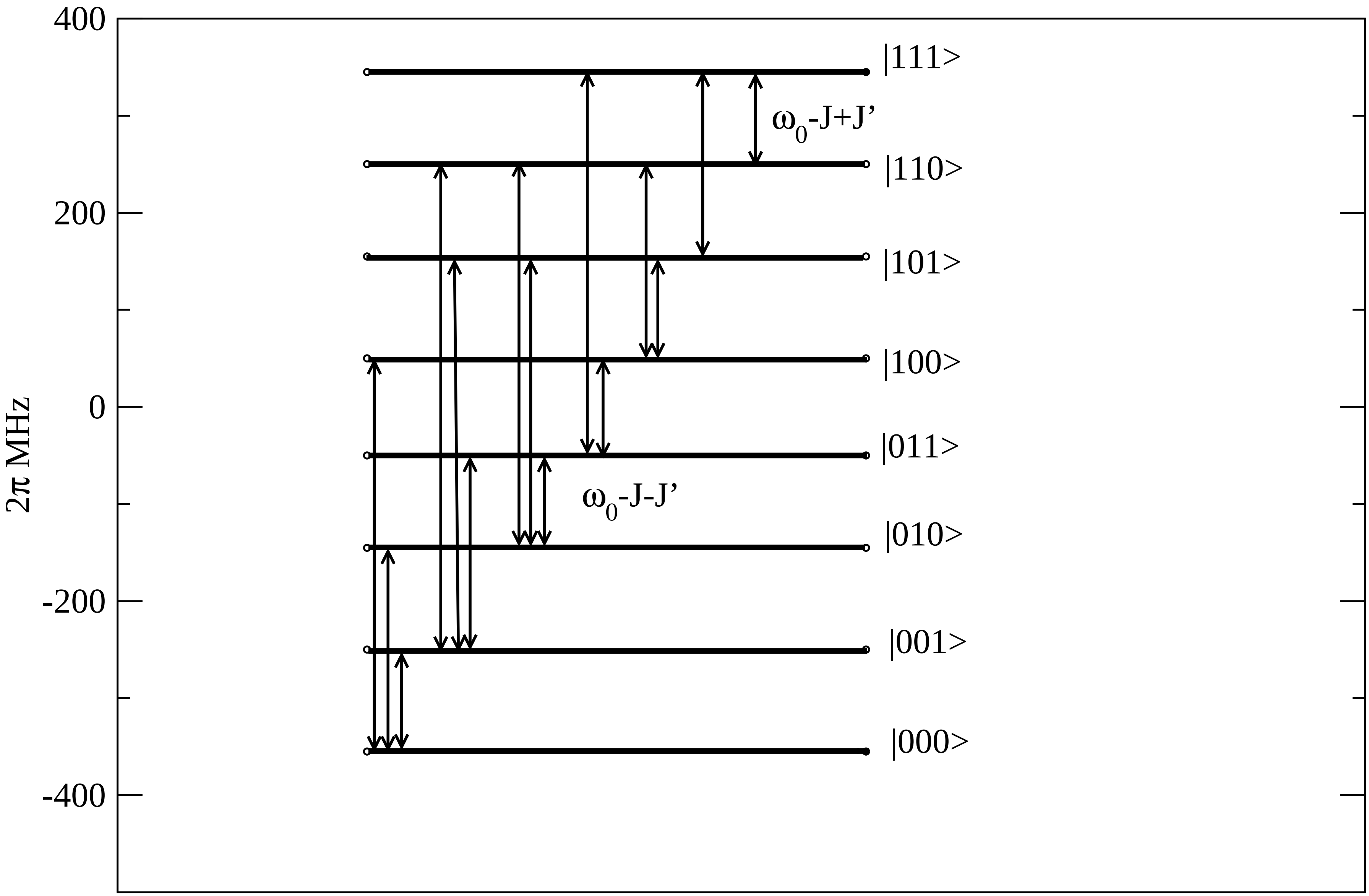
400
200
0
-200
-400
2π MHz
|111>
|110>
|101>
|100>
|011>
|010>
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ω0-J+J'
ω0-J-J'

Fig. 1

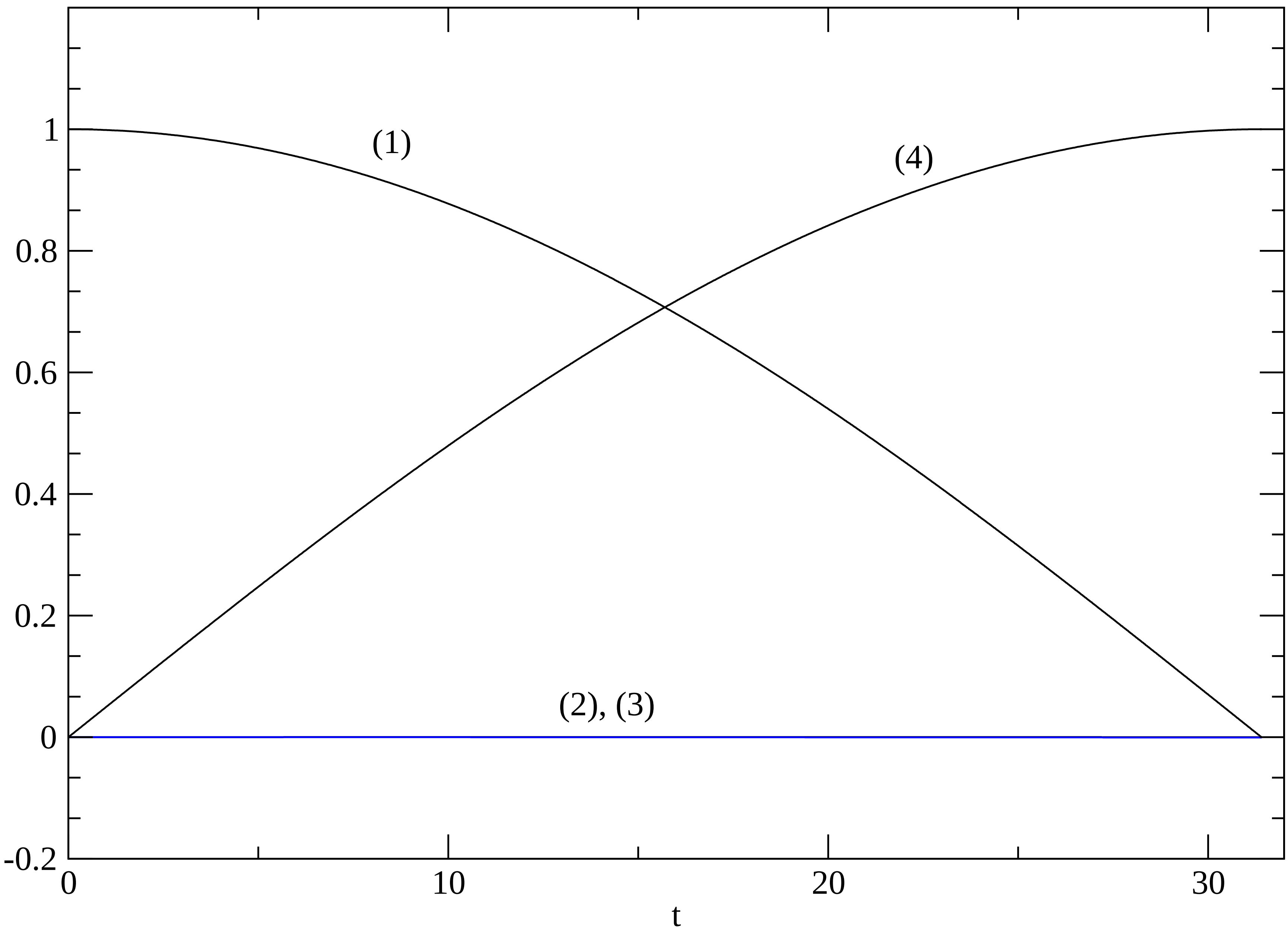

Fig. 2

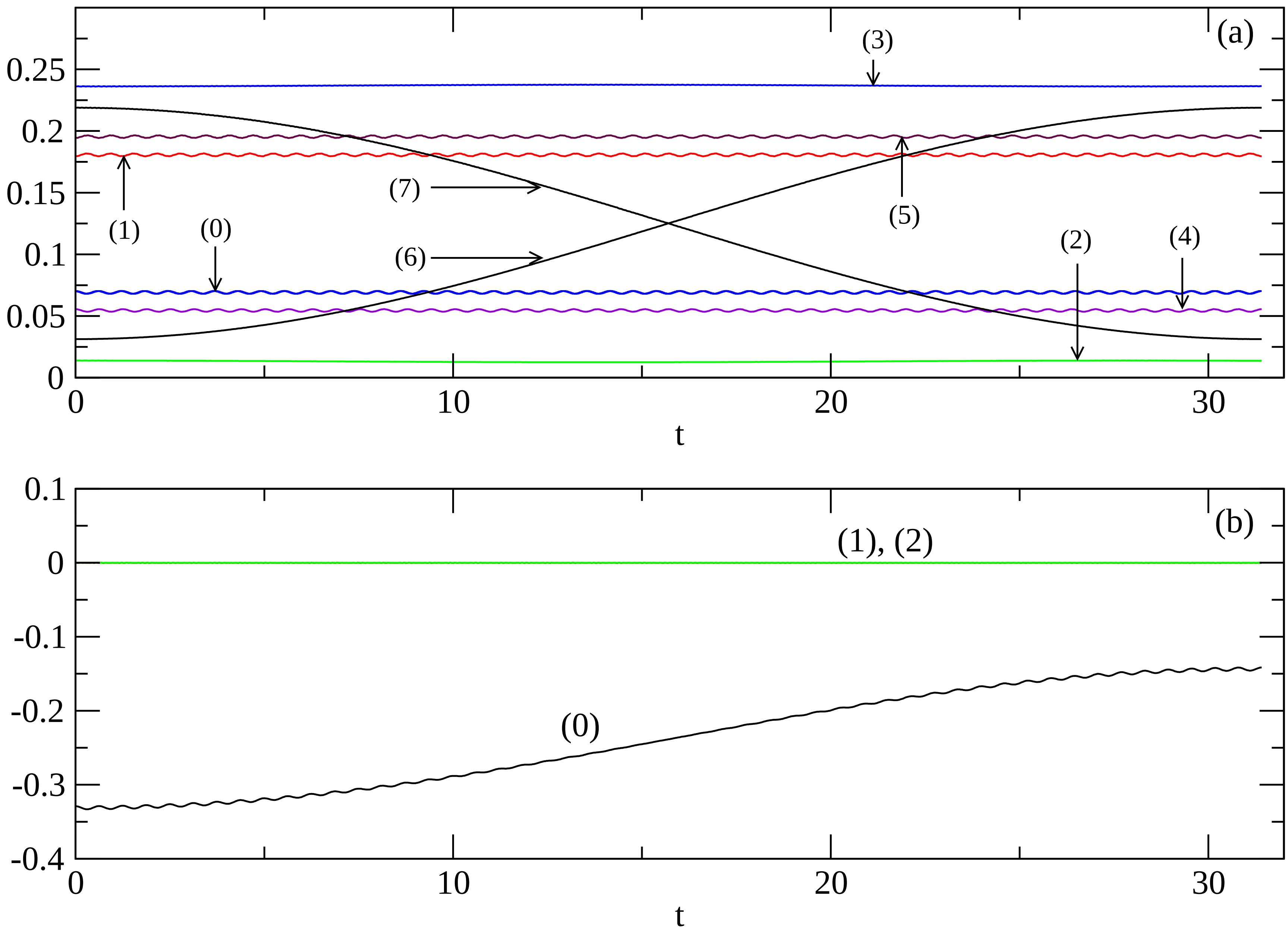
(a)
(3)
(7)
(1)
(0)
(6)
(5)
(2)
(4)
0.25
0.2
0.15
0.1
0.05
0
0
10
20
30
t
(b)
(1), (2)
(0)
0.1
0
-0.1
-0.2
-0.3
-0.4
0
10
20
30
t

Fig. 3

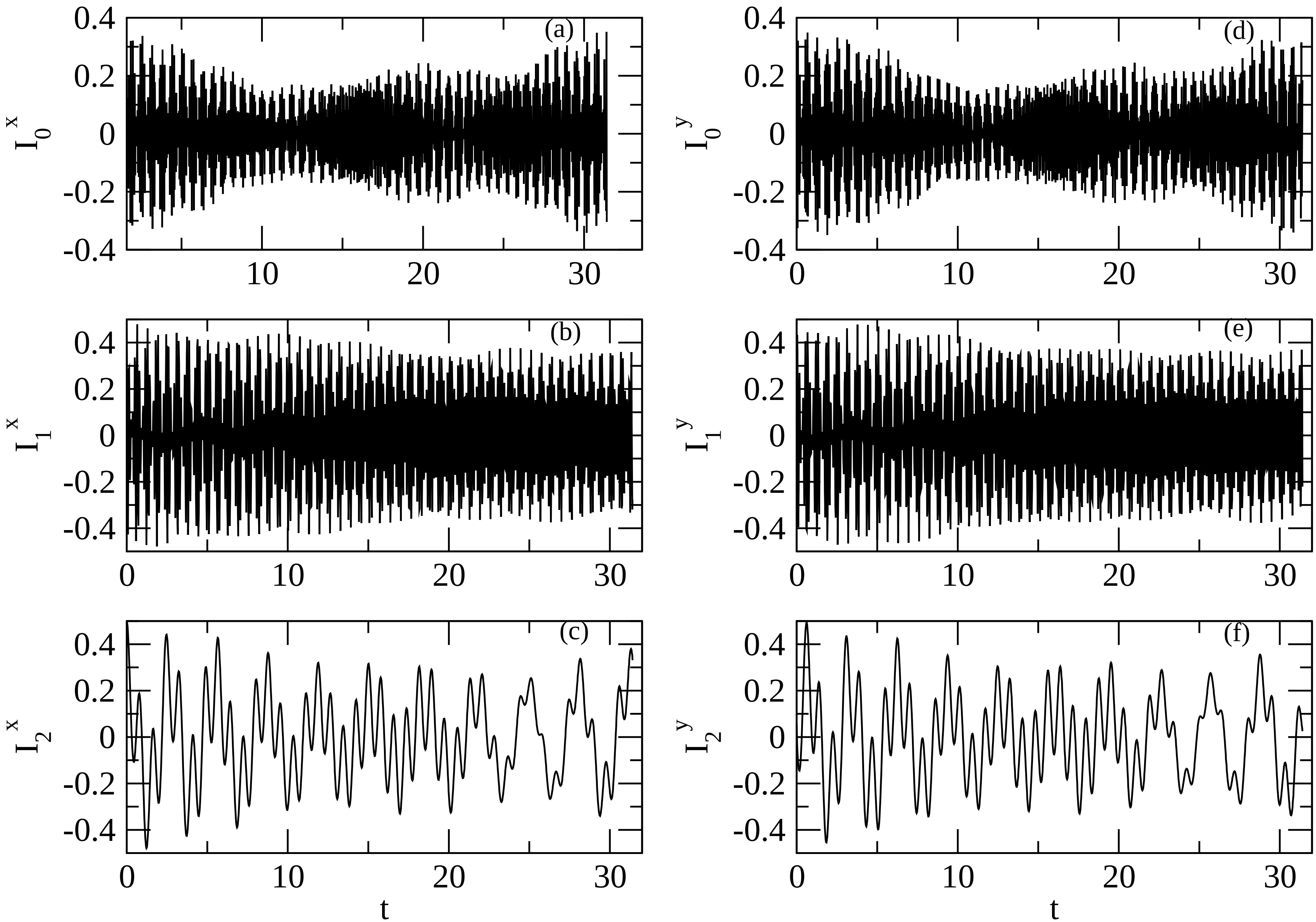

Fig. 4

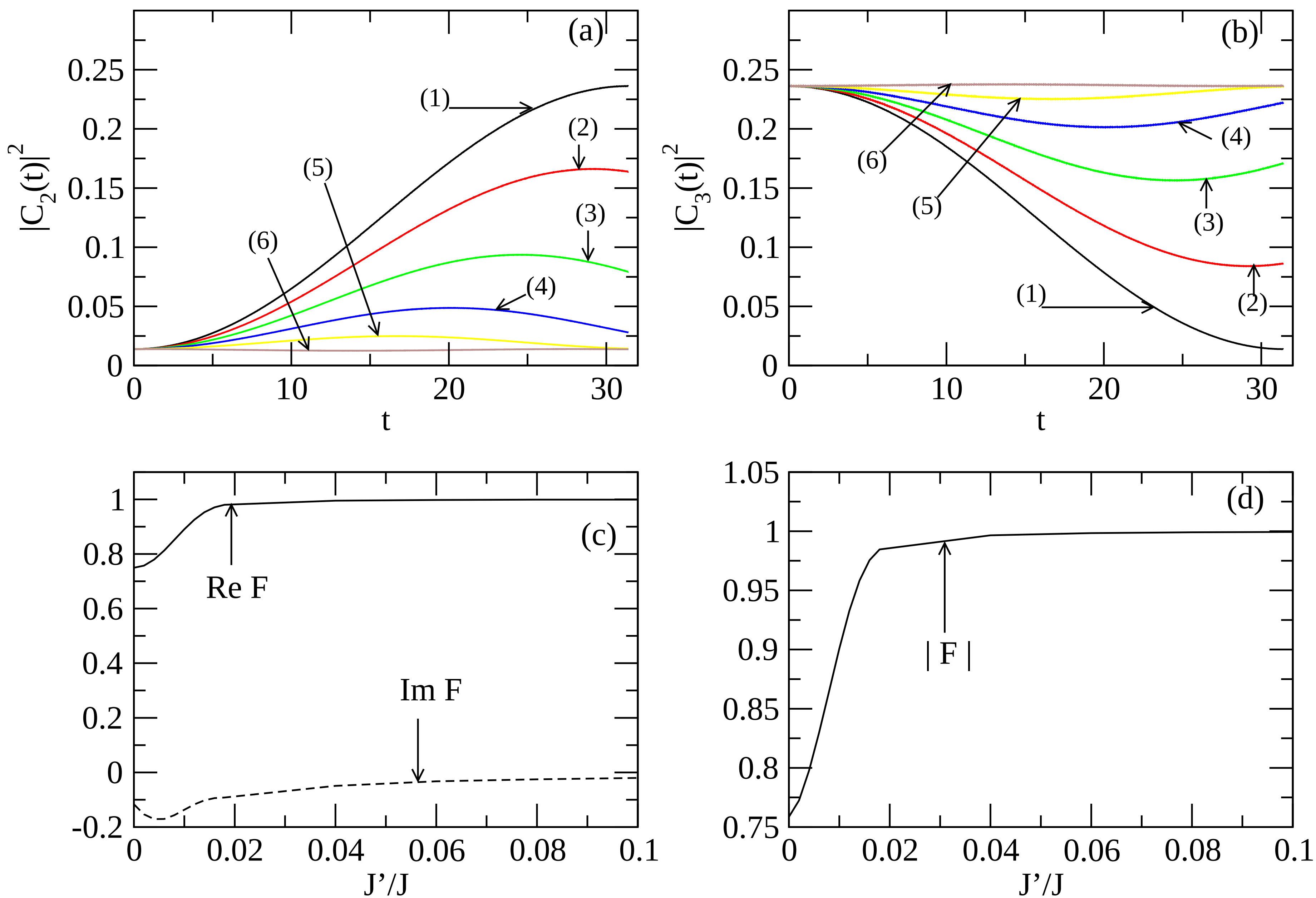

Fig. 5